1. Use the given dataset.
2. Apply pre-processing on dataset.
3. Convert SMILES string to atomic coordinate, substring, and molecular images.
4. Apply either of the GemNet, DimeNet, SczhNet model on all three granularity level.
5. See if some optimization is required or not.
6. See the performance metrics for all the granularity levels and compare via graphs

Reference for model
https://proceedings.neurips.cc/paper_files/paper/2021/hash/35cf8659cfcb13224cbd47863a34fc58-Abstract.html

https://arxiv.org/abs/2003.03123

https://scholar.google.com/scholar?hl=en&as_sdt=0%2C5&q=SchNet+architecture+&btnG=#d=gs_qabs&t=1696844789857&u=%23p%3Dp1xRFmplWJsJ